CHEMPHYSCHEM

Supporting Information

Spectroscopy and Redox Chemistry of Copper in Mordenite

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Supporting information

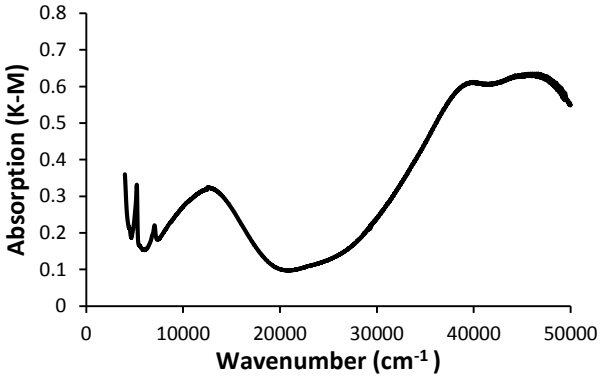


Figure S1: UV-vis-NIR spectrum of hydrated CuMOR sample ($CuMOR_{0.43}$).

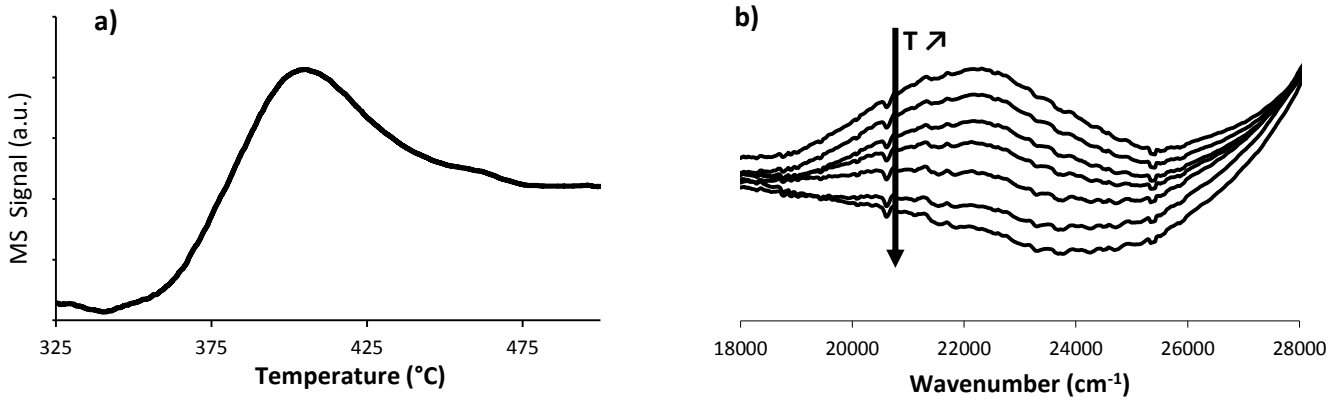


Figure S2: (A) Temperature programmed desorption (TPD) of O_2 after standard treatment and oxidation step at 250°C (rate 5°C/min). (B) Operando monitoring of the visible region during the TPD experiment.

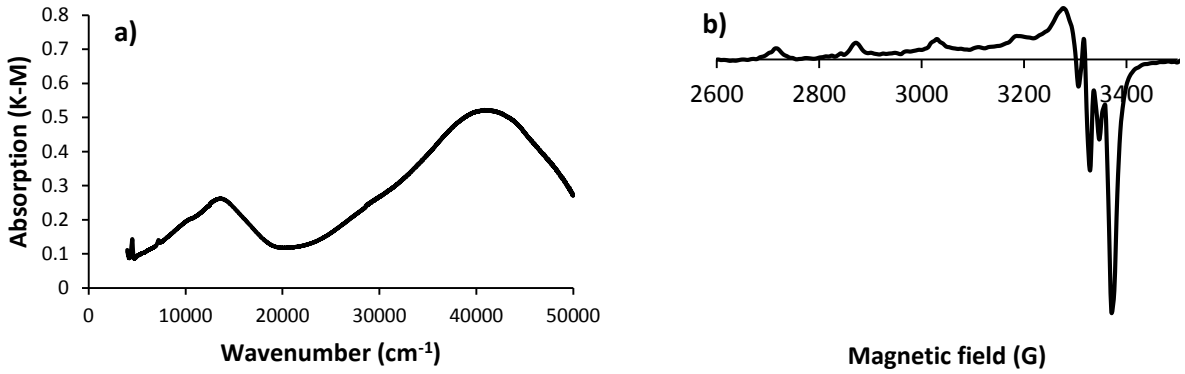
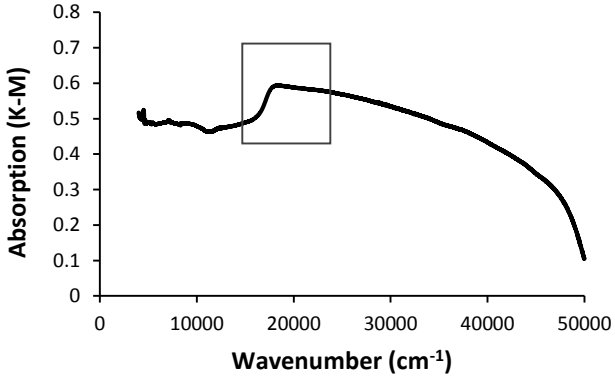


Figure S3: (A) UV-vis-NIR and (B) EPR spectrum of CuMOR sample ($CuMOR_{0.06}$) after standard treatment, *viz.* calcination in O_2 at 450°C followed by He treatment at 500°C.



FigureS4: UV-vis-NIR spectrum of CuMOR sample ($CuMOR_{0.43}$) after H_2 consumption peak at 400°C; the plasmon band can be observed at 18000 cm^{-1}.

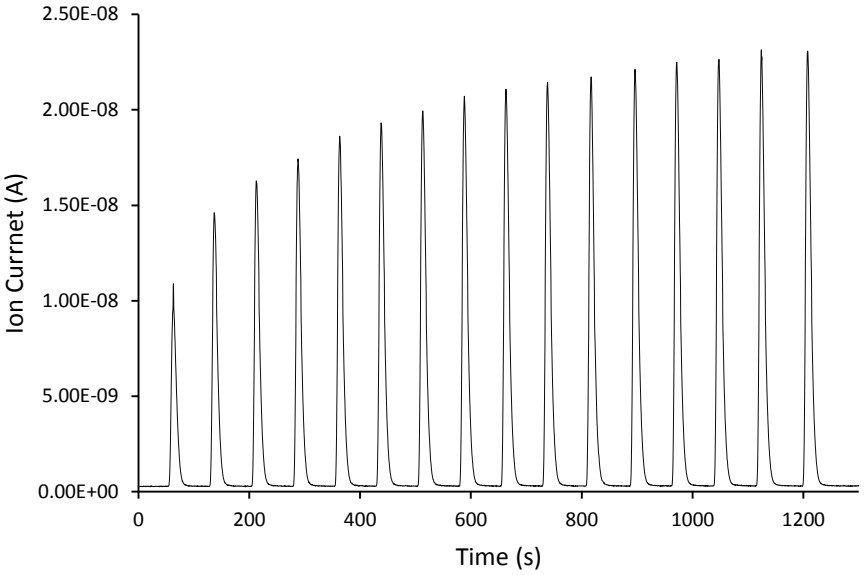


Figure S5: Quantification of H_2 consumption at 180°C of Cu-MOR sample (Cu-$MOR_{0.43}$) after standard treatment. H_2 pulses (frequency 0.8/min) were performed every 75s with a sample loop of 5µl.

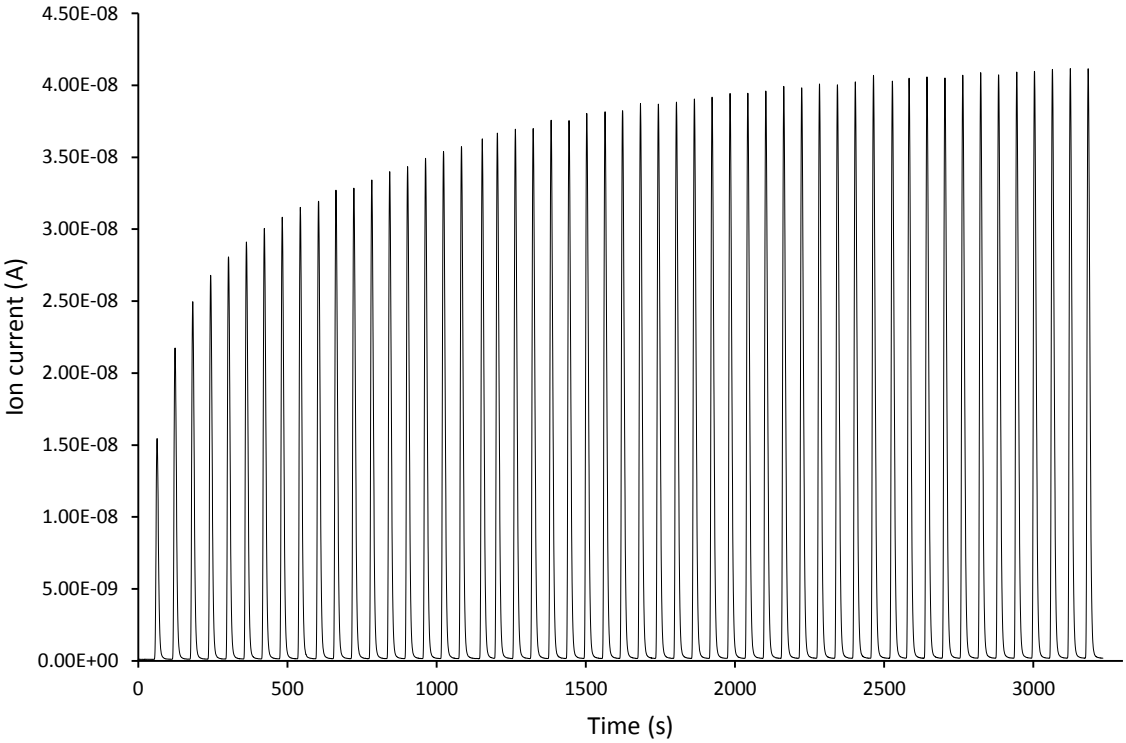


Figure S6: Quantification of H_2 consumption at 180°C of Cu-MOR sample (Cu-$MOR_{0.43}$) after standard treatment and extra oxidation at 250°C. H_2 pulses (frequency 1/min) were performed with a sample loop of 20µl.

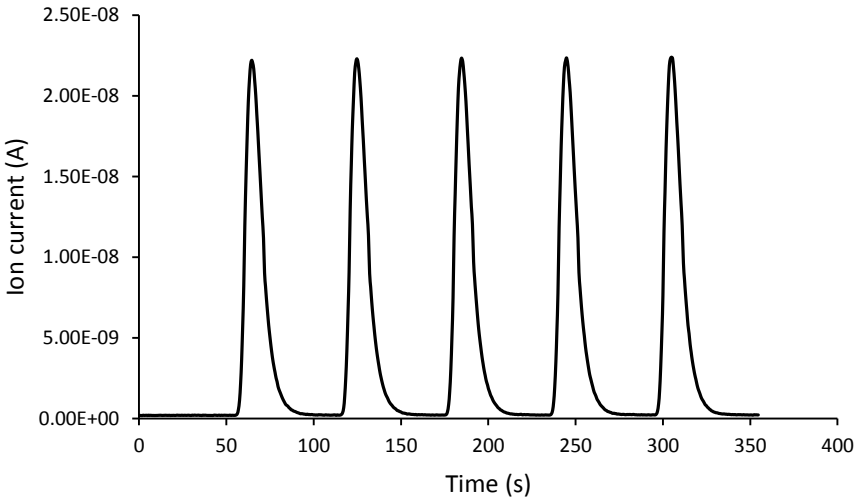


Figure S7: Quantification of H_2 consumption at 180°C of Cu-MOR sample (Cu-$MOR_{0.06}$) after standard treatment. H_2 pulses (frequency 1/min) were performed with a sample loop of 5µl.

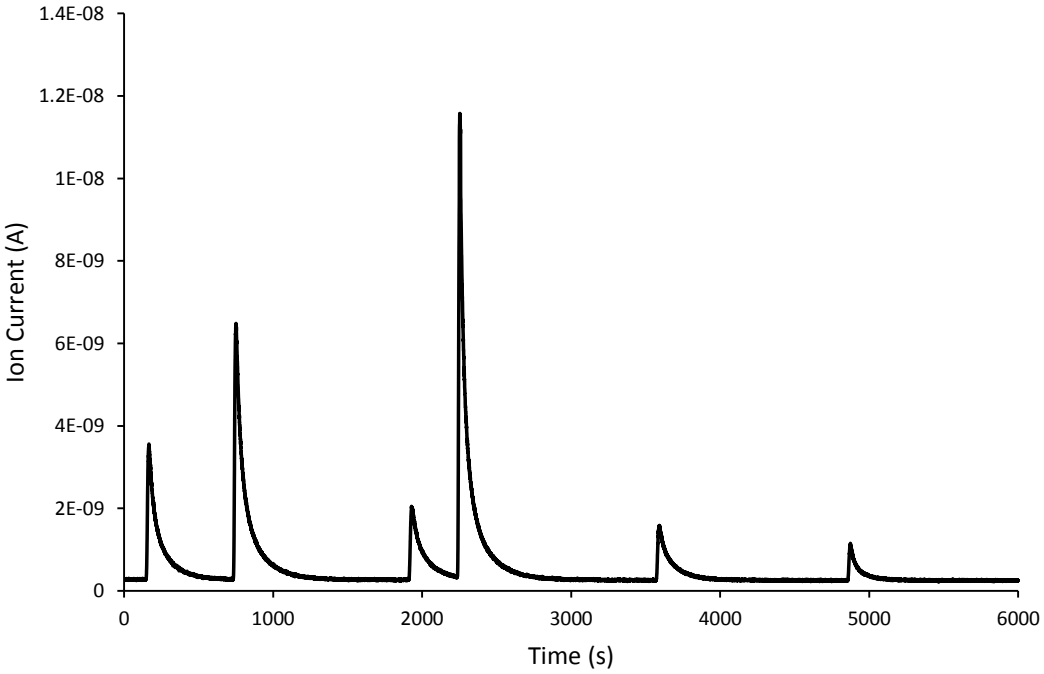


Figure S8: Example of H_2 pulses at 430°C on a Cu-MOR sample (Cu-$MOR_{0.43}$) after standard treatment. H_2 pulses were performed with a sample loop of 20µl.

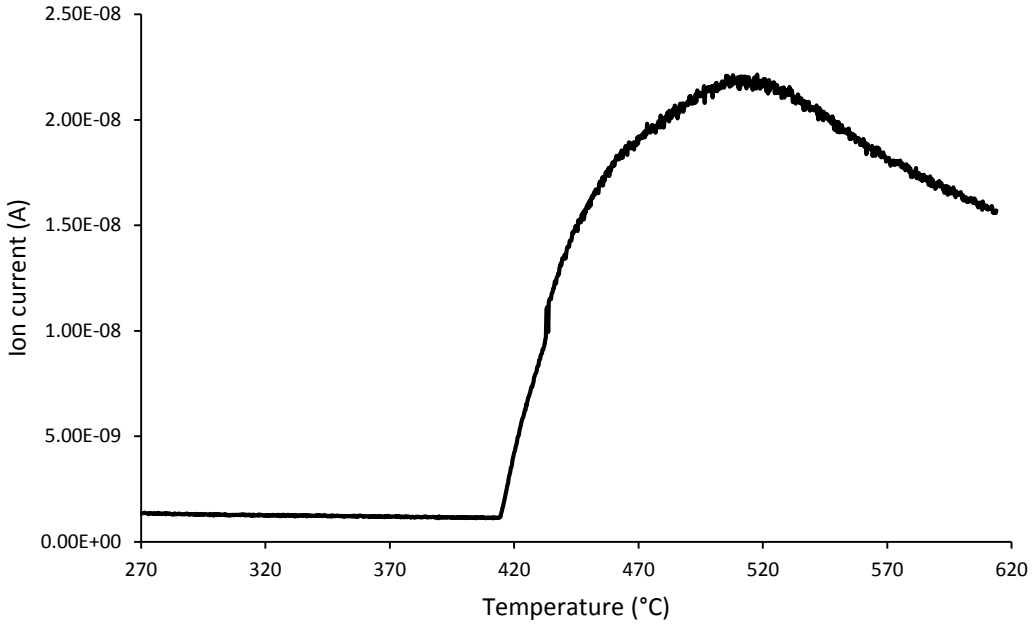


Figure S9: Water desorption in He flow (5°C/min) for a Cu-MOR sample (Cu-$MOR_{0.43}$) after the H_2 consumption peak at 180°C.

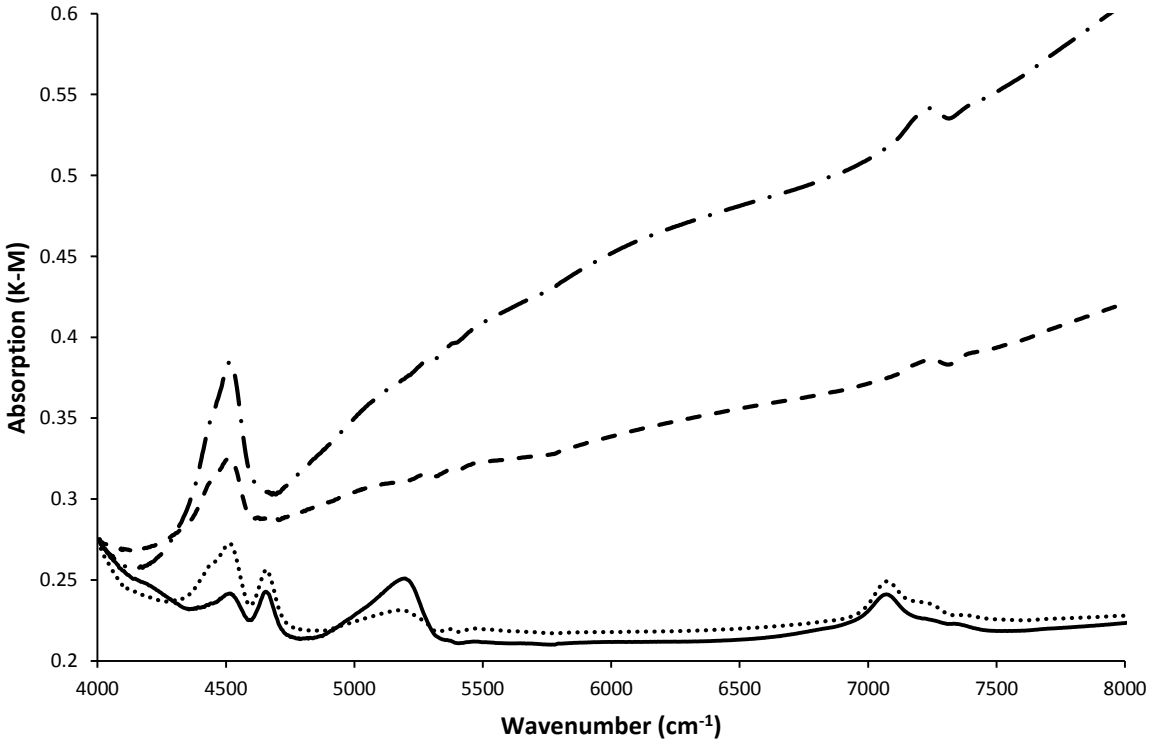


Figure S10: NIR spectrum of CuMOR sample (CuMOR$_{0.43}$) after standard treatment (– –) plus subsequent H2 reduction at 180°C (▪▪▪) and of an oxidized CuMOR sample (CuMOR$_{0.43}$) (▪ —) plus subsequent H2 reduction at 180°C (—). For both samples H_2 reduction at 180°C creates structural hydroxyl groups characterized by vibrations at 4660 cm^{-1} (ν+δ) and 7070 cm^{-1} (2ν). On the oxidized

sample there is a substantial amount of water formed by H_2 reduction at 180°C. This is evidenced by the vibration at 5200 cm^{-1} (ν+δ) characteristic for water.

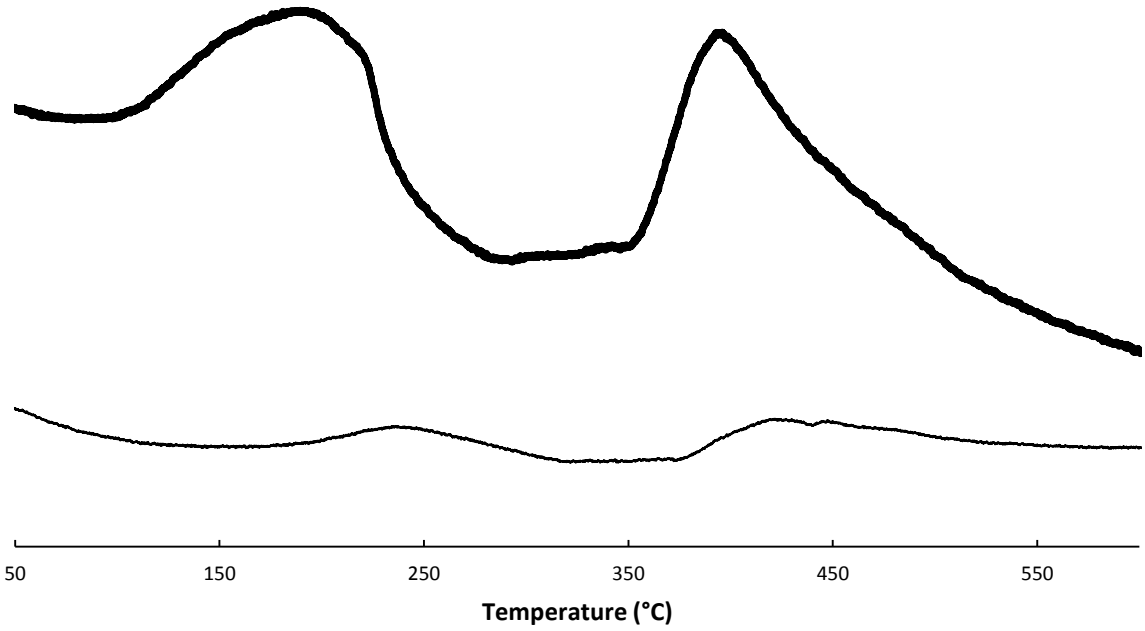


Figure S11: H_2 consumption during TPR of $CuMOR_{0.43}$ (bold line) and $CuMOR_{0.06}$ (thin line) after standard treatment.